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INVOLVING THE $(2p^2)^3P^e$ METASTABLE
AUTODETACHING OF H^-**

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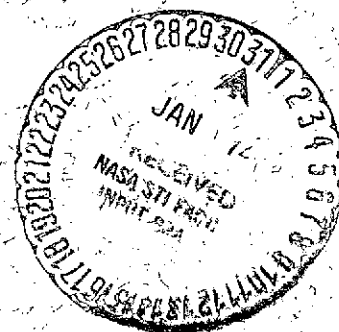
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RADIATIVE TRANSITIONS INVOLVING THE $(2p^2)^3P^e$
METASTABLE AUTODETACHING STATE OF H^-

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ABSTRACT

The absorption coefficient for the free-bound transition $H(1s) + e^- + h\nu \rightarrow H^-(2p^2, ^3P^e)$ is calculated (together with the differential emission rate for the inverse process) using $1s - 2s - 2p$ close coupling continuum wave functions and a Hylleraas bound state wave function. A maximum in the absorption and emission spectra is found to occur at a photon wavelength of 1219.5 \AA , which is 2 \AA closer to the Lyman α line than predicted by the calculations of Drake and is in closer agreement with the stellar absorption feature identified by Heap and Stecher. The free-bound absorption process appears to be a significant source of continuous ultraviolet opacity.

I. INTRODUCTION

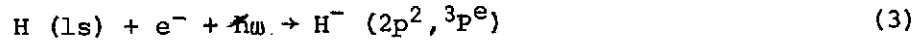
The continuous photoabsorption processes

$$\text{H}^- (1^1\text{S}) + \hbar\omega \rightarrow \text{H} (1\text{s}) + \text{e}^- \quad (1)$$

$$\text{H} (1\text{s}) + \text{e}^- + \hbar\omega \rightarrow \text{H} (1\text{s}) + \text{e}^- \quad (2)$$

play an important role in determining the visible and infrared opacities of stellar atmospheres. Elaborate variational calculations (Doughty, Fraser, and McEachran 1966; Doughty and Fraser 1966) indicate that the absorption coefficients are negligible at shorter wavelengths, but the contributions from the autodetaching resonances of H^- which can be excited by ultraviolet photons were not considered. For photodetachment from the H^- ground state, the autodetaching resonances are not expected to significantly enhance the absorption coefficient because they are the result of double-electron excitations. In the free-free transitions of H^- , however, the contributions from the final state resonances could be more significant and should be evaluated.

Within the LS-coupling approximation, the doubly excited $(2\text{p}^2)^3\text{p}^e$ state of H^- is bound by 0.0095 eV below the $\text{H} (2\text{p}) + \text{e}^-$ continuum threshold (Aashamar 1969, Drake 1970, Bhatia 1970). Because autodetachment into the $\text{H} (1\text{s}) + \text{e}^-$ continuum would violate conservation of either total orbital angular momentum or parity, the $(2\text{p}^2)^3\text{p}^e$ state may be described as a metastable autodetaching state. The close proximity of the $(2\text{p}^2)^3\text{p}^e$ state to the excitation threshold has led Heap and Stecher (1974) to attribute the broad stellar absorption feature which they have detected on the long-wavelength wing of the Lyman α line to the continuous (free-bound) absorption process.



Realistic variational calculations have been performed for the free-bound absorption coefficient (Drake 1974) as well as for the differential emission rate corresponding to the inverse (radiative decay) process (Drake 1973). However, the predicted spectra rise rapidly with increasing wavelength to a maximum value at 1221.5 Å, which is about 3 Å further from the Lyman α line than the observed absorption feature. In this paper, we report an independent calculation for the absorption and emission processes which indicates that the maximum occurs at 1219.5 Å, in closer agreement with the position of the observed spectral profile.

II. THEORY

The differential spontaneous emission rate for the $(2p^2) {}^3P^e \rightarrow (1s\,kp) {}^3P^o$ transition, which is the only possible electric-dipole decay mode for the $(2p^2) {}^3P^e$ state of H^- , is given in atomic units by

$$A(\omega) = \frac{4}{3} \frac{\omega^3}{c^3} \frac{\alpha^3}{3} \left| \langle 1s\,kp, {}^3P^o | \vec{r}_1 + \vec{r}_2 | 2p^2, {}^3P^e \rangle \right|^2 \quad (4)$$

where ω is the photon energy and α is the fine structure constant. The $(1s\,kp) {}^3P^o$ scattering continuum wave function is normalized per unit electron energy interval. The power radiated per unit volume per unit solid angle and angular frequency intervals is given by the emission coefficient:

$$\epsilon(\omega) = \frac{\hbar\omega}{4\pi} A(\omega) N_{H^-} \quad (5)$$

where N_{H^-} denotes the density of H^- ions in the $(2p^2)^3P^e$ state.

The effective absorption coefficient is defined in terms of the difference between absorption and stimulated emission and is given by

$$k(\omega) = \frac{4\pi^3 c^2}{\hbar \omega^3} \left(e^{\frac{\hbar\omega}{KT}} - 1 \right) \epsilon(\omega) \quad (6)$$

under the conditions of local thermodynamic equilibrium (Griem 1964).

With use of the Saha equation

$$\frac{N_H N_{e^-}}{N_{H^-}} = \frac{2 g_H}{g_{H^-}} \left(\frac{m KT}{2\pi\hbar^2} \right)^{3/2} e^{\frac{\Delta E}{KT}}, \quad (7)$$

where ΔE is the $H^- (2p^2, ^3P^e)$ energy measured from the hydrogen ground state, the expression for the absorption coefficient per unit hydrogen atom density per unit electron density (in units of a_0^5) may be written in the form

$$\alpha(\omega) = \frac{k(\omega)}{N_H N_{e^-}} = \frac{18 \pi^{7/2}}{(\alpha\omega)^2} \left(\frac{E_H}{KT} \right)^{3/2} \left(1 - e^{-\frac{\hbar\omega}{KT}} \right) e^{-\frac{E_{e^-}}{KT}} A(\omega) \quad (8)$$

E_H denotes the ionization energy of ground state atomic hydrogen, and the electron and photon energies are related by the energy conservation requirement.

$$E_{e^-} + \hbar\omega = \Delta E = 0.37465 \text{ a.u.} \quad (9)$$

equation (8) can also be derived from the expression for the free-free absorption coefficient corresponding to the transition to the final state continuum channel $H(2p) + e^-(\ell_2=1), {}^3P^e$. Except for our inclusion of stimulated emission, equation (8) is equivalent to the expression for the free-bound absorption coefficient derived independently by Drake (1974).

III. RESULTS AND DISCUSSION

In our evaluation of the differential spontaneous emission rate $A(\omega)$, the $(2p^2){}^3P^e$ state of H^- was represented by an 84 - term Hylleraas bound state wave function (Bhatia 1970), and the $(1s\ kp){}^3P^o$ scattering states were approximated by $1s$ - $2s$ - $2p$ close coupling continuum wave functions (Burke and Schey 1962). The length and the velocity forms of the dipole matrix element in equation (4) were evaluated over the allowed electron energy range using the procedures developed for photoionization calculations (Burke and McVicar 1965, Jacobs 1971). In contrast, Drake (1973) has evaluated $A(\omega)$ using a 50 - term Hylleraas function together with a discrete variational representation of and a free-electron approximation for the continuum.

The position and shape of the low electron energy spectral feature are found to be quite insensitive to the continuum approximation but are found to be surprisingly sensitive to the number N of Hylleraas terms included in the bound state wave function. The convergence of the differential emission rates obtained with three different expansions is nevertheless satisfactory when as many as 84 terms are included (figure 1). The length and velocity results presented over a more extended energy

range in Table 1 are in excellent agreement at low energies. For higher energies there is good agreement with the calculation of Drake (1973), but significant discrepancies are found near the maximum which are described below in connection with absorption.

The insensitivity to the continuum approximation is attributable to the fact that for very low electron energies the dominant contribution to the transition integral comes from large values of the ejected electron separation r where the continuum wave function may be represented by its asymptotic form. In addition, since the triplet P-wave phase shift tends to zero at threshold, it was expected and found that the Born approximation, i.e. replacement of the ejected electron continuum function by $j_1(Kr)$, gave essentially the same results as the more elaborate continuum functions. The same insensitivity to the continuum function was found by Drake (1973). The low electron energy variation of $A(\omega)$ is analogous to but much more rapid than the behavior of the H^- photodetachment absorption coefficient (Doughty, Fraser, and McEachran 1966), which also rises from zero at threshold to a maximum value.

In figure 2 our 84 - term results for the free-bound absorption coefficient per unit hydrogen atom density per unit electron density are compared with the absorption coefficient calculated by Drake (1974) for a temperature of 5000 K $^\circ$. We find a maximum at 1219.5 A $^\circ$ which is slightly larger and 2 A $^\circ$ closer to the Lyman α line than predicted by the calculation of Drake (1974). The variation of $\alpha(\omega)$ with temperature which is illustrated in Table 2 was an important consideration in

the identification of the $(2p^2)^3P^e$ state in the stellar absorption spectrum (Heap and Stecher 1974).

Drake (1974) has pointed out that for $Ne^- / N_H > 0.1$ the free-bound absorption coefficient per unit length is greater than that for Lyman α resonance broadening (Sando, Doyle, and Dalgarno 1969) in the wavelength interval $1220 \text{ \AA} - 1300 \text{ \AA}$. We wish to emphasize the dominance of the free-bound absorption process over the nonresonant free-free absorption process (Doughty and Fraser 1966) in the far ultraviolet, as illustrated by the comparison of the respective absorption coefficients given in figure 3.

A second maximum associated with the transition $H^- (2p^2, ^3P^e) \rightarrow H^- (2s \ 2p, ^3P^o) + h\nu$ is found to occur at a photon wavelength of 29, 138 \AA , corresponding to radiative decay via the $(2s \ 2p)^3P^o$ truly auto-detaching state of H^- . This far infrared emission feature is shown in figure 4. The peak value of $4.42 \times 10^9 \text{ sec}^{-1} \text{ a.u.}^{-1}$ is about 1/10 the maximum value in the far ultraviolet. Using a Hylleraas representation for the $(2s \ 2p)^3P^o$ resonance, a procedure which does not predict the resonant line shape, Drake (1973) has estimated that the inclusion of this transition increases the integrated decay rate by only about 1%. This autodetaching feature would in any event be suppressed in absorption because of the dominance of the nonresonant free-free transitions in the far infrared, but it might be observable in emission under non - LTE excitation conditions.

Additional sources of Lyman α resonance broadening absorption are expected from transitions to autodetaching resonances of H^- , several of

which are in close proximity to the $n = 2$ excitation threshold (Temkin and Walker 1965). Such contributions to the H^- free-free absorption coefficient could be as significant as that found for the $(2p^2)3p^e$ metastable autodetaching state, and calculations for all important resonances are in progress.

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TABLE 1

The differential spontaneous emission rate $A(\omega)$ (in units of $10^{10} \text{ sec}^{-1} \text{ a.u.}^{-1}$) for the transition $\text{H}^- (2p^2, ^3p^e) \rightarrow \text{H} (1s) + e^- + \hbar\omega$. The length and velocity results are denoted by L and V, respectively. The numbers in parenthesis are the powers of ten by which the entries are to be multiplied.

Electron energy (a.u.)	$A_L(\omega)$	$A_V(\omega)$
0.001	6.576	6.594
0.002	5.370	5.395
0.003	4.158	4.185
0.004	3.450	3.481
0.005	2.981	3.015
0.010	1.582	1.617
0.015	9.533 (-1)	1.005
0.020	6.400 (-1)	6.610 (-1)
0.025	4.332 (-1)	4.806 (-1)
0.030	3.122 (-1)	3.740 (-1)
0.040	1.976 (-1)	2.088 (-1)
0.050	1.212 (-1)	1.279 (-1)
0.100	1.727 (-2)	2.035 (-2)
0.150	4.153 (-3)	5.453 (-3)
0.200	1.311 (-3)	1.876 (-3)

TABLE 2

The free-bound absorption coefficient α (ω) (in units of cm^5). The numbers in parenthesis are the powers of ten by which the entries are to be multiplied.

λ (\AA)	$T = 5000 \text{ K}^\circ$	$T = 9000 \text{ K}^\circ$	$T = 1,5000 \text{ K}^\circ$
1216.9	6.49 (-38)	2.70 (-38)	1.26 (-38)
1217.7	1.17 (-37)	4.92 (-38)	2.30 (-38)
1218.6	1.41 (-37)	5.97 (-38)	2.80 (-38)
1219.4	1.46 (-37)	6.24 (-38)	2.94 (-38)
1220.2	1.42 (-37)	6.09 (-38)	2.88 (-38)
1221.0	1.33 (-37)	5.75 (-38)	2.73 (-38)
1221.8	1.23 (-37)	5.35 (-38)	2.55 (-38)
1222.7	1.13 (-37)	4.95 (-38)	2.36 (-38)
1224.3	9.60 (-38)	4.26 (-38)	2.05 (-38)
1225.9	8.28 (-38)	3.73 (-38)	1.80 (-38)
1229.2	6.50 (-38)	3.01 (-38)	1.48 (-38)
1232.6	5.32 (-38)	2.53 (-38)	1.26 (-38)
1249.5	2.13 (-38)	1.17 (-38)	6.26 (-39)
1266.8	9.62 (-39)	6.07 (-39)	3.48 (-39)
1284.7	4.83 (-39)	3.51 (-39)	2.15 (-39)
1303.1	2.57 (-39)	2.14 (-39)	1.41 (-39)
1322.0	1.41 (-39)	1.35 (-39)	9.61 (-40)
1361.5	4.56 (-40)	5.80 (-40)	4.72 (-40)

FIGURE CAPTIONS

Figure 1

The differential spontaneous emission rate $A(\omega)$ for the transition $H^- (2p^2, ^3P^e) \rightarrow H(1s) + e^- + \hbar\omega$ plotted as a function of the ejected electron energy and the emitted photon wavelength. N is the number of Hylleraas terms in the bound state wave function.

Figure 2

The free-bound absorption coefficient $\alpha(\omega)$ per unit hydrogen atom density per unit electron density for a temperature of 5000 K^o. The results of Drake (1974) are included for comparison.

Figure 3

The absorption coefficients for free-bound and free-free (Doughty and Fraser 1966) transitions of H^- for a temperature of 5000 K^o.

Figure 4

The resonant emission feature associated with the transition $H^- (2p^2, ^3P^e) \rightarrow H^- (2s\ 2p^3, ^3P^o) + \hbar\omega$ to the $(2s\ 2p)^3P^o$ autodetaching resonance of H^- .

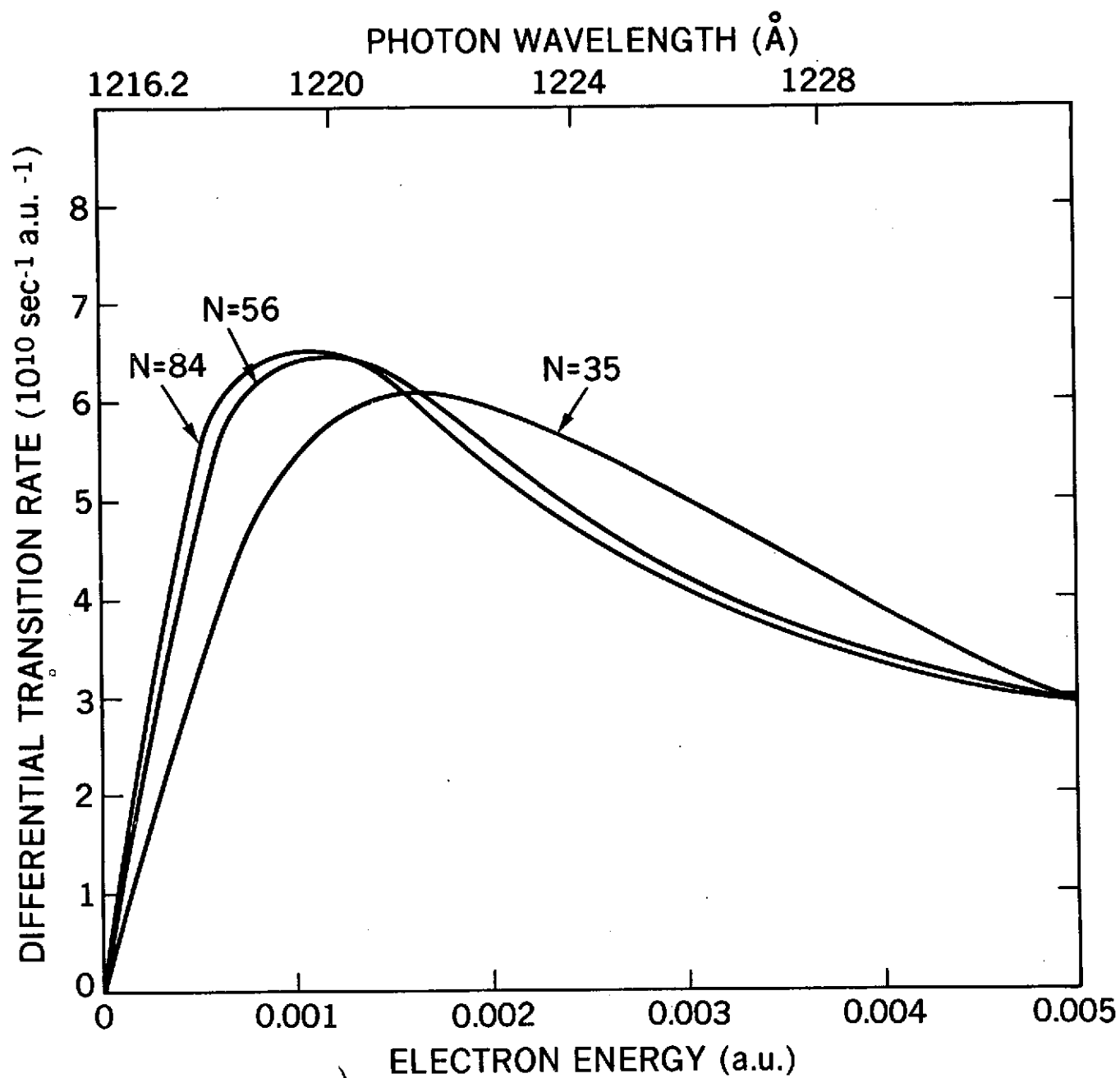


Figure 1

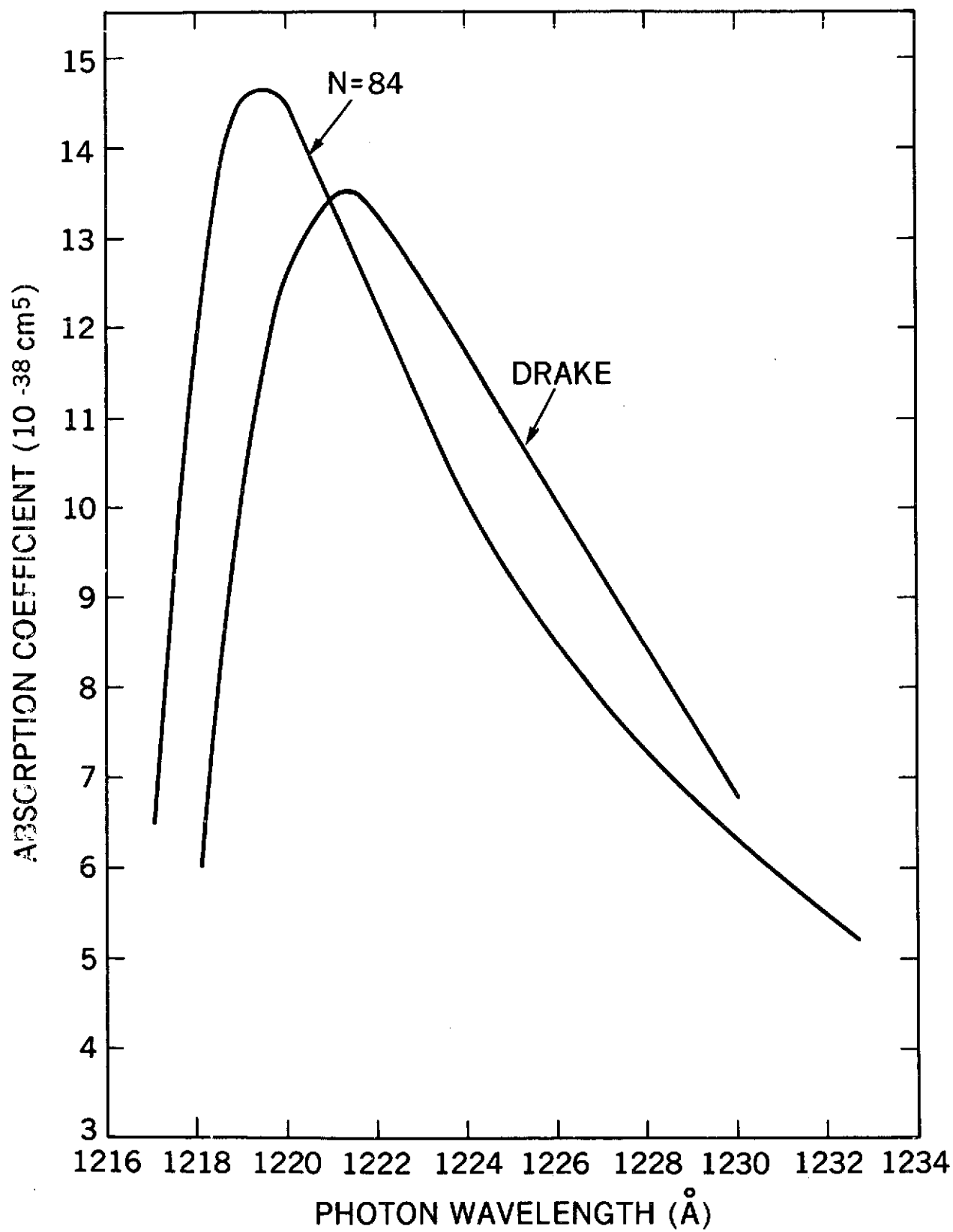


Figure 2

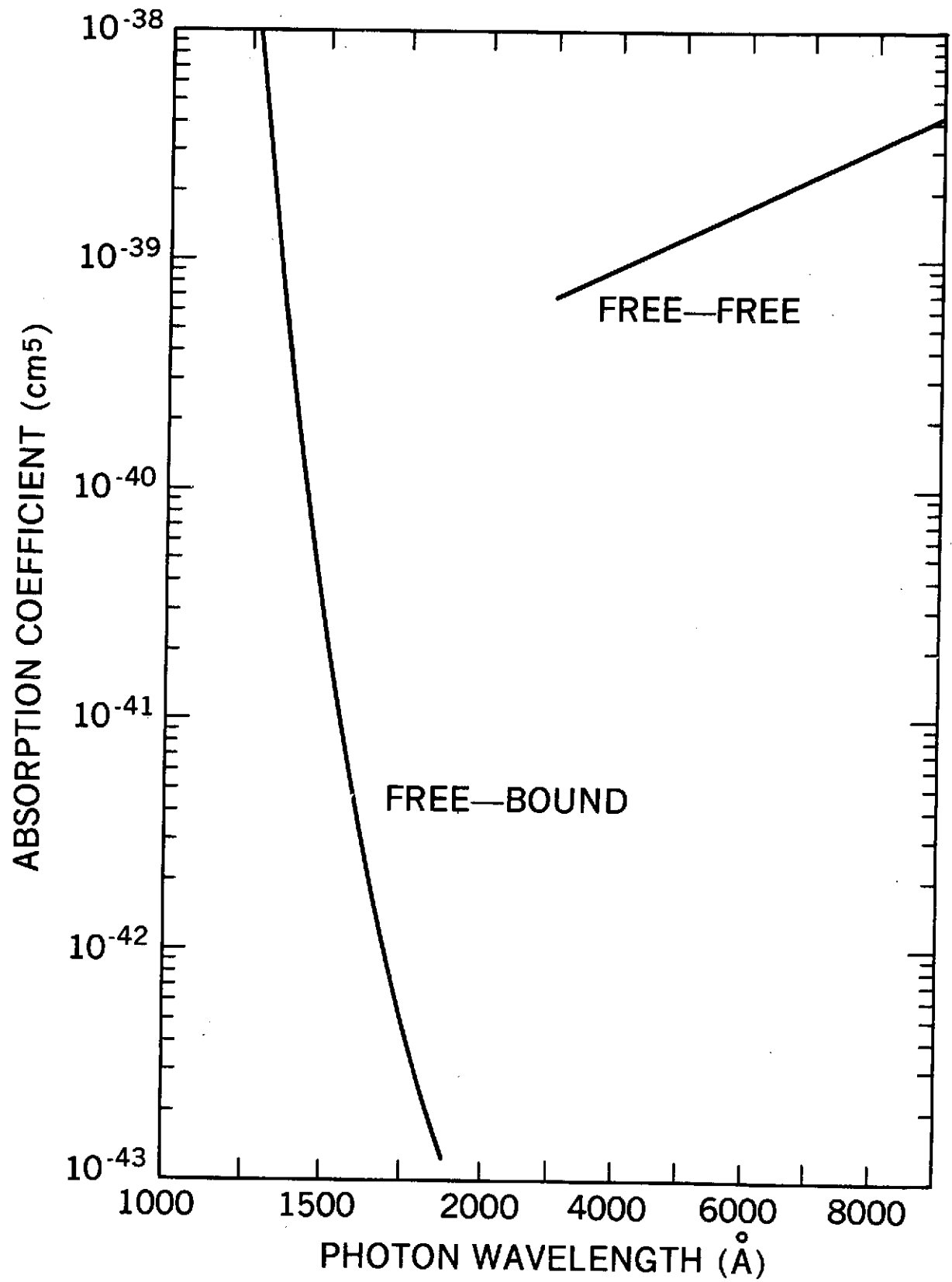


Figure 3

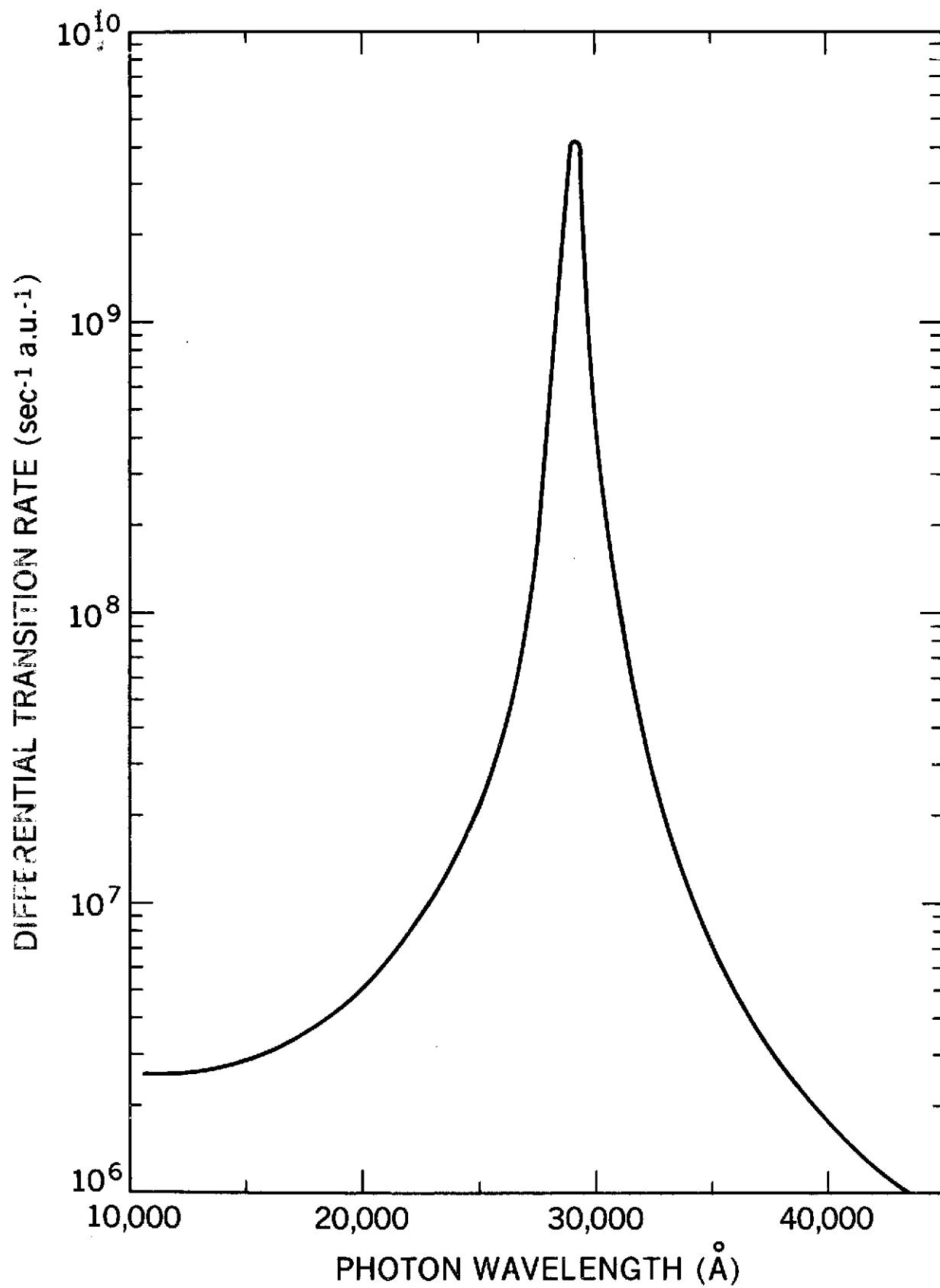


Figure 4.